WHAT IS CLAIMED IS:

1.   A system for analyzing a sample, comprising:

a liquid chromatograph into which the sample is input for chromatographic separation;

a mass spectrometer that receives the output of the liquid chromatograph and outputs a plurality of spectra of the sample at discrete times;

a computer coupled to the mass spectrometer wherein the computer receives the plurality of spectra and stores them in a two-dimensional data matrix;

a two-dimensional filter;

wherein the computer applies the two-dimensional filter to the data matrix to generate an output data matrix and examines the output data matrix to detect ions in the sample by identifying one or more peaks in the output data matrix.

2.   The system recited in claim 1, wherein the data matrix is configured such that each column of the data matrix corresponds to a distinct one of the plurality of spectra at a discrete time and each row of the data matrix corresponds to a chromatogram of the sample for a particular mass-to-charge ratio.

3.   The system recited in claim 1, wherein the peaks are detected by comparing each peak to a threshold and those peaks that exceed the threshold are deemed to be associated with ions.

4.   The system recited in claim 3, wherein the threshold is determined using a histogram of peak intensities.

5.   The system recited in claim 1, wherein the filter is a matched filter.

6.   The system recited in claim 1, wherein the filter is a rank-1 filter comprising a first filter that is convolved with the columns of the data matrix to generate a first intermediate matrix and a second filter that is convolved with the rows of the intermediate matrix to generate the output data matrix.

7.   The system recited in claim 6, wherein the rank-1 filter comprises one or more smoothing filters.

8.   The system recited in claim 6, wherein the rank-1 filter comprises one or more second derivative filters.

9.   The system recited in claim 1, wherein the filter is a rank-2 filter, comprising a first rank-1 filter and a second rank-1 filter, wherein the first rank-1 filter comprises a first filter that is convolved with the columns of the data matrix to generate

a first intermediate matrix and a second filter that is convolved with the rows of the first intermediate matrix to generated a second intermediate matrix, and the second rank-1 filter comprises a first filter that is convolved with the columns of the data matrix to generate a third intermediate matrix and a second filter that is convolved with the rows of the third intermediate matrix to generate a fourth intermediate matrix and wherein the second and fourth intermediate matrices are combined to generate the output data matrix.

10.   The system recited in claim 9, wherein the rank-2 filter comprises one or more smoothing filters.

11.   The system recited in claim 9, wherein the rank-2 filter comprises one or more second derivative filters.

12.   The system recited in claim 1, further comprising an ion list in which parameters corresponding to the ions are stored, wherein the parameters are determined by examining characteristics of the peaks in the output data matrix in an ion list.

13.   The system recited in claim 12, wherein the each row of the ion list comprises one or more parameters associated with a particular ion in the sample to which the row corresponds.

14.   The system recited in claim 13, wherein the one or more parameters comprise a mass-to-charge ratio associated with the particular ion, a retention time associated with the particular ion and an intensity associate with the particular ion.

15.   The system recited in claim 14 wherein the one or more parameters comprise characteristics of the peak.

16.   The system recited in claim 12, wherein the computer further produces a simplified spectrum or chromatogram by extracting related ions from the ion list to place in the simplified spectrum or chromatogram.

17.   The system recited in claim 16, wherein the related ions are chosen as those ions falling within a retention window.

18.   The system recited in claim 12, wherein the computer further produces a simplified chromatogram by extracting related ions from the ion list to place in the simplified spectrum.

19.   The system recited in claim 18, wherein the related ions are chosen as those ions falling within a mass-to-charge window.

20.   The system recited in claim 12, wherein one or more of the spectra are produced by modifying the mass spectrometer such that a set of spectra corresponding to the operation of the modified mass spectrometer are produced for analysis and a set of spectra corresponding to operation of the unmodified mass spectrometer are produced for analysis and a first ion list is generated for ions detected during operation of the unmodified mass spectrometer and a second ion list is generated for ions detected by operation of the modified mass spectrometer.

21.   The system recited in claim 20, wherein related ions in the first and second ion lists are identified by applying a retention time window to the first and second ions lists.

22.   The system recited in claim 20, wherein the modification is fragmentation switching.

23.   The system recited in claim 1, wherein the two-dimensional filter is applied to the data matrix by convolving the data matrix with the two-dimensional filter.

24.   A method for analyzing a sample, comprising:

introducing the sample into a liquid chromatograph for chromatographic separation to a liquid chromatograph output;

introducing the liquid chromatograph output into a mass spectrometer that outputs a plurality of mass spectra of the sample at discrete times;

inputting two or more of the plurality of mass spectra into a computer;

storing the two or more mass spectra in a two-dimensional data matrix;

specifying a two-dimensional filter to apply to the data matrix;

applying the two-dimensional filter to the data matrix to generate an output data matrix; and

examining the output data matrix to detect ions in the sample by identifying one or more peaks in the output data matrix, wherein each peak corresponds to an ion in the sample.

25.   The method recited in claim 24, further comprising configuring the data matrix such that each column of the data matrix corresponds to a distinct one of the plurality of spectra at a discrete time and each row of the data matrix corresponds to a chromatogram of the sample for a particular mass-to-charge ratio.

26.   The method recited in claim 24, further comprising:

comparing each peak to a detection threshold; and

identifying those peaks that those peaks that satisfy the detection threshold as peaks associated with detected ions.

27. The method recited in claim 26, further comprising:

creating a histogram of peak intensities from the data matrix; and

determining the detection threshold in accordance with the histogram.

28. The method recited in claim 24, wherein the two-dimensional filter is a matched filter.

29. The method recited in claim 24, further comprising:

specifying a rank-1 filter comprising a first filter and a second filter;

convolving the columns of the data matrix with the first filter to generate a first intermediate matrix; and

convolving the rows of the intermediate matrix with the second filter to generate the output data matrix.

30. The method recited in claim 29, wherein the rank-1 filter comprises one or more smoothing filters.

31. The method recited in claim 29, wherein the rank-1 filter comprises one or more second derivative filters.

32. The method recited in claim 24, further comprising:

specifying a rank-2 filter, comprising a first rank-1 filter and a second rank-1 filter, wherein the first rank-1 filter comprises a first filter and a second filter and the second rank-1 filter comprises a third filter and a fourth filter;

convolving the columns of the data matrix with the first filter to generate a first intermediate matrix;

convolving the rows of the first intermediate matrix with the second filter to generate a second intermediate matrix;

convolving the columns of the data matrix with the third filter to generate a third intermediate matrix;

convolving the rows of the third intermediate matrix with the fourth filter to generate a fourth intermediate matrix;

combining the second and fourth matrices to generate the output data matrix.

33. The method recited in claim 32, wherein the rank-2 filter comprises one or more smoothing filters.

34.   The method recited in claim 32, wherein the rank-2 filter comprises one or more second derivative filters.

35.   The method recited in claim 24, further comprising:

examining characteristics of the peaks identified as corresponding to detected ions to obtain parameters corresponding to the detected ions; and

storing the parameters corresponding to the detected ions in an ion list.

36.   The method recited in claim 35, wherein the each row of the ion list comprises one or more parameters associated with a particular ion in the sample to which the row corresponds.

37.   The method recited in claim 35, wherein the one or more parameters comprise a mass-to-charge ratio associated with the particular ion, a retention time associated with the particular ion and an intensity associate with the particular ion.

38.   The method recited in claim 37, wherein the one or more parameters comprise characteristics of the peak.

39.   The method recited in claim 35, further comprising extracting related ions from the ion list to create a simplified spectrum or chromatogram.

40.   The method recited in claim 39, further comprising:

specifying a retention time window; and

identifying related ions from the ion parameter list as those ions having retention times falling within the retention time window.

41.   The method recited in claim 39, wherein the computer further produces a simplified chromatogram by extracting related ions from the ion list to place in the simplified spectrum.

42.   The method recited in claim 41, further comprising:

specifying a mass-to-charge ratio window; and

identifying related ions from the ion parameter list as those ions having mass-to-charge ratios falling within the mass-to-charge ratio window.

43.   The method recited in claim 35, further comprising:

generating a set of spectra corresponding to the operation of the mass spectrometer for analysis;

storing a first ion parameter list for ions detected during operation of the mass spectrometer;

modifying the mass spectrometer;

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generating a set of spectra corresponding to the operation of the modified mass spectrometer for analysis; and

storing a second ion parameter list for ions detected during operation of the modified mass spectrometer.

44. The method recited in claim 43, further comprising:

specifying a retention time window; and

identifying related ions from the first and second ion parameter list as those ions having retention times falling within the retention time window.

45. The method recited in claim 43, wherein the modification is fragmentation switching.

46. The method recited in claim 24, further comprising convolving the data matrix with the filter.

47. A system for analyzing a sample, comprising:

means for introducing the sample into a liquid chromatograph for chromatographic separation to a liquid chromatograph output;

means for introducing the liquid chromatograph output into a mass spectrometer that outputs a plurality of mass spectra of the sample at discrete times;

means for inputting two or more of the plurality of mass spectra into a computer;

means for storing the two or more mass spectra in a two-dimensional data matrix;

means for specifying a two-dimensional filter to apply to the data matrix;

means for applying the two-dimensional filter to the data matrix to generate an output data matrix; and

means for examining the output data matrix to detect ions in the sample by identifying one or more peaks in the output data matrix, wherein each peak corresponds to an ion in the sample.

48. The method recited in claim 47, further comprising means for configuring the data matrix such that each column of the data matrix corresponds to a distinct one of the plurality of spectra at a discrete time and each row of the data matrix corresponds to a chromatogram of the sample for a particular mass-to-charge ratio.

49. The method recited in claim 47, further comprising:

means for comparing each peak to a detection threshold; and

means for identifying those peaks that those peaks that satisfy the detection threshold as peaks associated with detected ions.

50.   The method recited in claim 49, further comprising:

means for creating a histogram of peak intensities from the data matrix; and

means for determining the detection threshold in accordance with the histogram.

51.   The method recited in claim 47, wherein the two-dimensional filter is a matched filter.

52.   The method recited in claim 47, further comprising:

means for specifying a rank-1 filter comprising a first filter and a second filter;

means for convolving the columns of the data matrix with the first filter to generate a first intermediate matrix; and

means for convolving the rows of the intermediate matrix with the second filter to generate the output data matrix.

53.   The method recited in claim 52, wherein the rank-1 filter comprises one or more smoothing filters.

54.   The method recited in claim 52, wherein the rank-1 filter comprises one or more second derivative filters.

55.   The method recited in claim 47, further comprising:

means for specifying a rank-2 filter, comprising a first rank-1 filter and a second rank-1 filter, wherein the first rank-1 filter comprises a first filter and a second filter and the second rank-1 filter comprises a third filter and a fourth filter;

means for convolving the columns of the data matrix with the first filter to generate a first intermediate matrix;

means for convolving the rows of the first intermediate matrix with the second filter to generate a second intermediate matrix;

means for convolving the columns of the data matrix with the third filter to generate a third intermediate matrix;

means for convolving the rows of the third intermediate matrix with the fourth filter to generate a fourth intermediate matrix;

means for combining the second and fourth matrices to generate the output data matrix.

56.   The method recited in claim 55, wherein the rank-2 filter comprises one or more smoothing filters.

57.   The method recited in claim 55, wherein the rank-2 filter comprises one or more second derivative filters.

58.   The method recited in claim 47, further comprising:

means for examining characteristics of the peaks identified as corresponding to detected ions to obtain parameters corresponding to the detected ions; and

means for storing the parameters corresponding to the detected ions in an ion list.

59.   The method recited in claim 58, wherein the each row of the ion list comprises one or more parameters associated with a particular ion in the sample to which the row corresponds.

60.   The method recited in claim 58, wherein the one or more parameters comprise a mass-to-charge ratio associated with the particular ion, a retention time associated with the particular ion and an intensity associate with the particular ion.

61.   The method recited in claim 60, wherein the one or more parameters comprise characteristics of the peak.

62.   The method recited in claim 58, further means for comprising extracting related ions from the ion list to create a simplified spectrum or chromatogram.

63.   The method recited in claim 62, further comprising:

means for specifying a retention time window; and

means for identifying related ions from the ion parameter list as those ions having retention times falling within the retention time window.

64.   The method recited in claim 62, wherein the computer further produces a simplified chromatogram by extracting related ions from the ion list to place in the simplified spectrum.

65.   The method recited in claim 64, further comprising:

means for specifying a mass-to-charge ratio window; and

means for identifying related ions from the ion parameter list as those ions having mass-to-charge ratios falling within the mass-to-charge ratio window.

66.   The method recited in claim 58, further comprising:

means for generating a set of spectra corresponding to the operation of the mass spectrometer for analysis;

means for storing a first ion parameter list for ions detected during operation of the mass spectrometer;

means for modifying the mass spectrometer;

means for generating a set of spectra corresponding to the operation of the modified mass spectrometer for analysis; and

means for storing a second ion parameter list for ions detected during operation of the modified mass spectrometer.

67.   The method recited in claim 66, further comprising:

means for specifying a retention time window; and

means for identifying related ions from the first and second ion parameter list as those ions having retention times falling within the retention time window.

68.   The method recited in claim 66, wherein the modification is fragmentation switching.

69.   The method recited in claim 47, further comprising means for convolving the data matrix with the filter.